

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Leslie Wong Examiner #: 68866 Date: 3/30/04
 Art Unit: 1761 Phone Number 303-2-1411 Serial Number: 09/541624
 Mail Box and Bldg/Room Location: RTM18A151 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

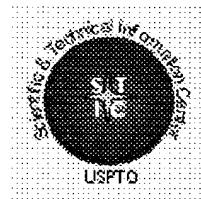
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	Type of Search	Vendors and cost where applicable
Searcher: <u>E.L.</u>	NA Sequence (#)	STN <u>\$ 237.32</u>
Searcher Phone #: _____	AA Sequence (#)	Dialog _____
Searcher Location: _____	Structure (#)	<u>(2)</u> Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic	<u>(and)</u> Dr. Link _____
Date Completed: <u>4-1-04</u>	Litigation	Lexis/Nexis _____
Searcher Prep & Review Time: <u>5</u>	Fulltext	Sequence Systems _____
Clerical Prep Time: _____	Patent Family	WWW/Internet _____
Online Time: <u>70</u>	Other	Other (specify) _____



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Name:

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Class / Subclass(es)

Earliest Priority Filing Date:

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Provide detailed information on your search topic:

- In your own words, describe in detail the concepts or subjects you want us to search.
- Include synonyms, keywords, and acronyms. Define terms that have special meanings.
- *For Chemical Structure Searches Only*
Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers
- *For Sequence Searches Only*
Include all pertinent information (parent, child, divisional, or issued patent numbers) along with

the appropriate serial number.

- *For Foreign Patent Family Searches Only*
Include the country name and patent number.
- Provide examples or give us relevant citations, authors, etc., if known.
- FAX or send the **abstract, pertinent claims** (not all of the claims), **drawings, or chemical structures** to your EIC or branch library.

Enter your Search Topic Information below:

Compound of Formula I as attached in claim 1 as a flavor or fragrance. Specifically compounds of claims 2 and 3.

I already have the compound but it is not used as a flavor or fragrance (GB 1409209).

Special Instructions and Other Comments:

(For fastest service, let us know the best times to contact you, in case the searcher needs further clarification on your search.)

Press ALT + F, then P to print this screen for your own information.

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Last Modified: 12/05/2003 15:08:46

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=> display history full 11-

FILE 'LREGISTRY' ENTERED AT 18:55:09 ON 01 APR 2004
L1 STR

FILE 'HCAPLUS' ENTERED AT 18:59:17 ON 01 APR 2004
L2 91 SEA GASSENMEIER ?/AU
L3 352 SEA GRAB ?/AU
L4 36 SEA GALOPIN ?/AU
L5 368 SEA BIGLER ?/AU
L6 0 SEA L2 AND L3 AND L4 AND L5
L7 3 SEA L2 AND L3
L8 0 SEA L2 AND L4
L9 0 SEA L2 AND L5
L10 0 SEA L3 AND L4
L11 0 SEA L3 AND L5
L12 0 SEA L4 AND L5
D L7 1-3 TI
SEL L7 1-3 RN

FILE 'REGISTRY' ENTERED AT 19:02:53 ON 01 APR 2004
L13 174 SEA (123-51-3/BI OR 124-13-0/BI OR 127-91-3/BI OR
L14 12 SEA L13 AND C H O S/ELF

FILE 'LREGISTRY' ENTERED AT 19:05:18 ON 01 APR 2004
L15 STR

FILE 'REGISTRY' ENTERED AT 19:07:12 ON 01 APR 2004
L16 3 SEA SSS SAM L15
L17 469 SEA SSS FUL L15
SAV L17 WON624/A
L18 7 SEA SUB=L17 SSS SAM L1
L19 STR L1
L20 0 SEA SUB=L17 SSS SAM L19
L21 13 SEA SUB=L17 SSS FUL L19
SAV L21 WON624A/A

FILE 'CAOLD' ENTERED AT 19:11:44 ON 01 APR 2004
L22 1 SEA L21
L23 28 SEA L17

FILE 'HCAPLUS' ENTERED AT 19:12:21 ON 01 APR 2004

L24 19 SEA L21
L25 356 SEA L17
L26 149834 SEA (FRAGRAN? OR PERFUM? OR PARFUM? OR COLOGNE? OR ODOR?
OR AROMA# OR SMELL? OR SCENT? OR OLFACT? OR REDOLENT? OR
ESSENCE? OR BOUQUET? OR AMBROS? OR ORGANOLEP?)/BI,AB
L27 206166 SEA (FLAVOR? OR FLAVOUR? OR SAVOR? OR SAVOUR? OR SAPID?
OR SAPOR? OR TAST? OR PALAT? OR GUSTAT? OR TOOTHSOME? OR
DELECTAB? OR SEASON? OR SPICE? OR APPETIZ? OR ORGANOLEP?)
/BI,AB
L28 917464 SEA (MIXT# OR MIXTURE? OR BLEND? OR ADMIX? OR COMMIX? OR
IMMIX? OR INTERMIX? OR COMPOSIT? OR COMPN# OR COMPSN# OR
FORMULAT? OR INTERSPER?)/TI

FILE 'LCA' ENTERED AT 19:13:31 ON 01 APR 2004

L29 15216 SEA (MIX? OR BLEND? OR ADMIX? OR COMMIX? OR IMMIX? OR
INTERMIX? OR DOPE# OR DOPING# OR DOPANT? OR IMPREGNAT?
OR COMPOSIT? OR COMPN# OR COMPSN# OR FORMULAT? OR
COMBINAT? OR INTERSPER? OR AMALGAM?)/BI,AB

FILE 'HCAPLUS' ENTERED AT 19:14:02 ON 01 APR 2004

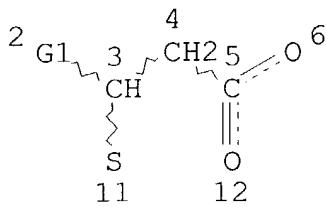
L30 16571 SEA (L26 OR L27) (2A) L29
L31 5 SEA L24 AND L26
L32 2 SEA L24 AND L27
L33 9 SEA L25 AND L26
L34 5 SEA L25 AND L27
L35 0 SEA (L31 OR L32) AND L28
L36 1 SEA (L31 OR L32) AND L30
L37 0 SEA (L33 OR L34) AND L28
L38 2 SEA (L33 OR L34) AND L30
L39 5 SEA L36 OR L31 OR L32
L40 6 SEA (L33 OR L34 OR L38) NOT L39

FILE 'CAOLD' ENTERED AT 19:17:00 ON 01 APR 2004

L41 27 SEA L23 NOT L22

FILE 'REGISTRY' ENTERED AT 19:18:03 ON 01 APR 2004

=> d 121 que stat
L15 STR



VAR G1=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU

NODE ATTRIBUTES:

CONNECT IS X2 RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

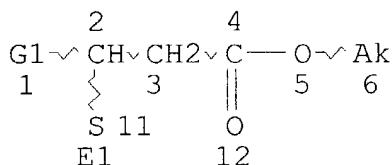
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L17 469 SEA FILE=REGISTRY SSS FUL L15

L19 STR



VAR G1=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU

NODE ATTRIBUTES:

HCOUNT IS E1 AT 11

CONNECT IS E1 RC AT 6

CONNECT IS E1 RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X8 C AT 6

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L21 13 SEA FILE=REGISTRY SUB=L17 SSS FUL L19

100.0% PROCESSED 273 ITERATIONS

SEARCH TIME: 00.00.01

13 ANSWERS

=> file caold

FILE 'CAOLD' ENTERED AT 19:18:24 ON 01 APR 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

=> d 122 1 all hitstr

L22 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN

AN CA53:2092c CAOLD

TI quaternary ammonium compds.

AU Ploetz, Ernst

PA Badische Anilin- & Soda-Fabrik Akt.-Ges.

DT Patent

PATENT NO.	KIND	DATE
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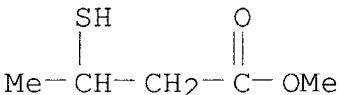
PI DE 944130

IT 54051-19-3 98560-63-5

IT 54051-19-3 98560-63-5

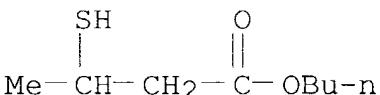
RN 54051-19-3 CAOLD

CN Butanoic acid, 3-mercaptop-, methyl ester (9CI) (CA INDEX NAME)



RN 98560-63-5 CAOLD

CN Butyric acid, 3-mercaptop-, butyl ester (6CI) (CA INDEX NAME)



=> d 141 1-27 ti

L41 ANSWER 1 OF 27 CAOLD COPYRIGHT 2004 ACS on STN

TI relations between the Cu atoms of ceruloplasmin - (I) studies on the exchange of ^{64}Cu with ceruloplasmin, (II) interaction between the Cu binding sites

L41 ANSWER 2 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI synthesis of some potential antiradiation agents - (II) 1,3-thiazane derivs.

L41 ANSWER 3 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiochromone synthesis

L41 ANSWER 4 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI quaternary distilbazole compds.

L41 ANSWER 5 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI 7-sulfamidothiachroman 1,1-dioxides

L41 ANSWER 6 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI reaction of α -amino acids with acrylamide

L41 ANSWER 7 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiochromones with schistosomicide activity

L41 ANSWER 8 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI reaction of thiourea with α -bromobutyric acid - (II)
peculiarities of the reaction at low concn. of starting materials

L41 ANSWER 9 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI ion-exchange chromatography of S amino acids and the sepn. of diastereoisomers

L41 ANSWER 10 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiophosphoric acid esters and pesticidal compns.

L41 ANSWER 11 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI quick-acting chem. balance

L41 ANSWER 12 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI addn. of mercaptoketones to reactive double bonds - (III) reactions with unsatd. carbonyl compds. and acid derivs.

L41 ANSWER 13 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI 3,3'-thioether dicarboxylic acids and their esters

L41 ANSWER 14 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI app. for the detn. in vacuo of the elec. cond. and Hall coeff. of thin metallic films and semiconductors
TI countercurrent distribution method for sepn. of chem. compds.

L41 ANSWER 15 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI photographic emulsions, antifogging agents for

L41 ANSWER 16 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI S-contg. amino acid

L41 ANSWER 17 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI antituberculous S compds. - (I) mercapto derivs. of alkanols, sulfides, and hydroxy sulfides

L41 ANSWER 18 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI Dieckmann reaction-prepn. of thiophenone derivs.

L41 ANSWER 19 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI phosphorothiolothionates from esters of alkene- and alkane-1,1-diols

L41 ANSWER 20 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI dithiophosphoric esters (heterocyclic)
TI heterocyclic dithiophosphoric esters

L41 ANSWER 21 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI synthesis of α - and β - (6-purinylthio)carboxylic acids

L41 ANSWER 22 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI β -thioethers of aliphatic aldehydes

L41 ANSWER 23 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI mineral acid salts of substituted isothiourea compds.

L41 ANSWER 24 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI antimetabolites - (I) synthesis and properties of sulfonic acid analogs of δ -aminolevulinic acid

L41 ANSWER 25 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI stabilization of poly(vinyl acetals)

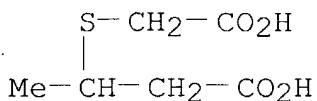
L41 ANSWER 26 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI flavor problem of soybean oil - (XIII) S coordination compds. effective in edible-oil stabilization

L41 ANSWER 27 OF 27 CAOLD COPYRIGHT 2004 ACS on STN
TI thiazole series - (III) S-heterocyclic derivs. of 2-aminothiazole

=> d 141 26 all hitstr

L41 ANSWER 26 OF 27 CAOLD COPYRIGHT 2004 ACS on STN

AN CA51:7607g CAOLD
 TI flavor problem of soybean oil - (XIII) S coordination compds.
 effective in edible-oil stabilization
 AU Schwab, Arthur W.; Moser, H. A.; Gurley, R. S.; Evans, C. D.
 IT 99-68-3 111-17-1 123-93-3 505-47-5 **4386-05-4**
 5961-83-1 67242-91-5 92473-81-9 105910-65-4 119641-92-8
 IT **4386-05-4**
 RN 4386-05-4 CAOLD
 CN Butanoic acid, 3-[(carboxymethyl)thio]- (9CI) (CA INDEX NAME)



=> file hcplus
 FILE 'HCPLUS' ENTERED AT 19:19:53 ON 01 APR 2004
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 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d 139 1-5 ibib abs hitstr hitind

L39 ANSWER 1 OF 5 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2001:798002 HCPLUS
 DOCUMENT NUMBER: 135:343645
 TITLE: Preparation and use of ethyl 3-mercaptopropionate
 as a **flavoring or fragrance**
 agent
 INVENTOR(S): Dewis, Mark Lawrence; Edwards, David John;
 Kendrick, Lesley; Wright, Maria
 PATENT ASSIGNEE(S): International Flavors + Fragrances Inc., USA
 SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001080666	A1	20011101	WO 2001-US12518	20010417
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GE, HU, IN, IS, JP, KE, KG, KP, KR, KZ, LK, LR,				

LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO,
 RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN,
 AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD,
 TG

GB 2363964 A1 20020116 GB 2000-9769 20000419
 EP 1276390 A1 20030122 EP 2001-927136 20010417

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC,
 PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2002150662 A1 20021017 US 2001-7095 20011204
 US 2004037787 A1 20040226 US 2003-645772 20030821

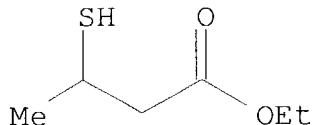
PRIORITY APPLN. INFO.: GB 2000-9769 A 20000419
 WO 2001-US12518 W 20010417
 US 2001-7095 B3 20011204

AB Et 3-mercaptopropionate may be used in a wide variety of ingestible vehicles such as chewing gum compns., hard and soft confections, beverages, etc., to impart a green, mango, fruity **odor**. It may also be used in a **perfuming compn.** or a **perfumed article** as an active **perfuming** ingredient. Et 3-mercaptopropionate is prep'd. by reaction of Et crotonate with sodium hydrogen sulfide and sodium bicarbonate to form the disulfide dimer of Et 3-mercaptopropionate followed by reducing the disulfide dimer to yield Et 3-mercaptopropionate.

IT 156472-94-5P
 (prepn. and use of Et 3-mercaptopropionate as a **flavoring** or **fragrance** agent)

RN 156472-94-5 HCPLUS

CN Butanoic acid, 3-mercaptopro-, ethyl ester (9CI) (CA INDEX NAME)



IC ICM A23L001-22
 CC 17-6 (Food and Feed Chemistry)
 Section cross-reference(s): 23, 62
 ST mercaptobutyrate ethyl **flavoring fragrance**
 IT Air fresheners
 Beverages
 Chewing gum
Colognes
 Confectionery
 Deodorants

Fabric softeners
 Flavoring materials
 Odor and Odorous substances
 Perfumes
 Shampoos
 (Et mercaptobutyrate as a **flavoring** or
fragrance agent)
 IT Soaps
 (Et mercaptobutyrate as a **flavoring** or
fragrance agent)
 IT Bath preparations
 (gels; Et mercaptobutyrate as a **flavoring** or
fragrance agent)
 IT Detergents
 (household cleaners; Et mercaptobutyrate as a **flavoring**
 or **fragrance** agent)
 IT Detergents
 (laundry; Et mercaptobutyrate as a **flavoring** or
fragrance agent)
 IT Mango (Mangifera indica)
 (prepn. and use of Et mercaptobutyrate as a **flavoring**
 or **fragrance** agent)
 IT 156472-94-5P
 (prepn. and use of Et mercaptobutyrate as a **flavoring**
 or **fragrance** agent)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN
 THE RE FORMAT

L39 ANSWER 2 OF 5 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2000:742586 HCPLUS
 DOCUMENT NUMBER: 134:16811
 TITLE: Quantitative Determination of Sulfur Containing
 Wine **Odorants** at Sub-ppb Levels. 1.
 Synthesis of the Deuterated Analogues
 AUTHOR(S): Kotseridis, Yorgos; Ray, Jean-Loiec; Augier,
 Christian; Baumes, Raymond
 CORPORATE SOURCE: Unite Biopolymeres Aromes, INRA-IPV,
 Montpellier, 34060, Fr.
 SOURCE: Journal of Agricultural and Food Chemistry
 (2000), 48(12), 5819-5823
 CODEN: JAFCAU; ISSN: 0021-8561
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB [2H10]-4-Sulfanyl-4-methylpentan-2-one (d10-SMP),
 [2H2]-3-sulfanylhexan-1-ol (d2-3SH), and [2H5]-3-sulfanylhexyl
 acetate (d5-3SHAc), the labeled analogs of impact **odorants**

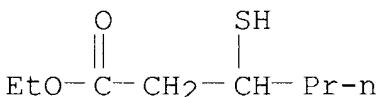
of wines and other foods, were synthesized to be used for the quant. detn. of the natural compds. in white and red wines by stable isotope diln. assay. The sulfidation was achieved by Michael addn., on mesityl oxide or Et hex-2-enoate, resp., of the sulfhydryl anion generated in situ from triphenylsilanethiol and potassium fluoride under phase transfer conditions. The labeling of 4-sulfanyl-4-methylpentan-2-one (SMP) was obtained from the com. starting material, [2H6]acetone, so that this method could be used to synthesize 13C-labeled SMP from 13C-labeled acetone. The labeling of 3-sulfanylhexan-1-ol (3SH) and 3-sulfanylhexyl acetate (3SHAc) was obtained from redn. with lithium aluminum deuteride of the Michael adduct Et 3-sulfanylhexanoate and [2H3]-acetylation. During the synthesis, 3SH and 3SHAc were partially oxidized to their disulfide, which were reduced back to the thiols by an addnl. redn. step; the tertiary thiol SMP was less sensitive to this oxidn.

IT 309250-83-7

(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

RN 309250-83-7 HCPLUS

CN Hexanoic acid, 3-mercaptop-, ethyl ester (9CI) (CA INDEX NAME)



CC 17-11 (Food and Feed Chemistry)

ST sulfur compd wine **odorant** deuterated detn

IT Deuteriation

Odor and Odorous substances

Wine analysis

(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

IT 309250-80-4P 309250-81-5P 309250-82-6P

(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

IT 7789-23-3, Potassium fluoride 17455-13-9, 18-Crown-6 ether

(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

IT 128-37-0, 2,6-Di-tert-butyl-p-cresol, reactions 141-79-7, Mesityl oxide 1552-67-6, Ethyl hex-2-enoate 7704-34-9D, Sulfur, compds., reactions 14128-54-2, Lithium aluminum deuteride 14606-42-9, Triphenylsilanethiol 19872-52-7 51755-83-0 309250-83-7

(quant. detn. of sulfur contg. wine **odorants** at sub-ppb levels, synthesis of deuterated analogs)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE

IN THE RE FORMAT

L39 ANSWER 3 OF 5 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1985:565917 HCPLUS
 DOCUMENT NUMBER: 103:165917
 TITLE: Hair removal and waving with mercaptoisobutyric acid
 INVENTOR(S): Pfleiderer, Ernst; Taeger, Tilman; Ude, Werner;
 Wick, Gertrud
 PATENT ASSIGNEE(S): Rohm G.m.b.H., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 27 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3339104	A1	19850509	DE 1983-3339104	19831028

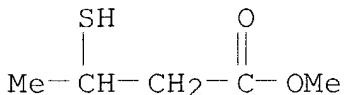
PRIORITY APPLN. INFO.: DE 1983-3339104 19831028

AB Cosmetic depilatories, hide dehairing prepns., and cold waving solns. contain β -mercaptoisobutyric acid [26473-47-2], its salts, and/or esters, and/or compds. that form these compds. in alk. medium. The hair prepns. contain 5-70 g active compd./100 mL liq. and have a pH of 6-13. A liq. depilatory contained Me β -mercaptoisobutyrate [54051-19-3] 100, CM-cellulose 3, propylene glycol 115, EtoH 42, perfume oil 10, and H2O 700 g.

IT 54051-19-3
 (cosmetic depilatories and waving prepns. and hide dehairing prepns. contg.)

RN 54051-19-3 HCPLUS

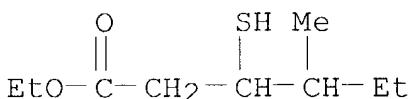
CN Butanoic acid, 3-mercapto-, methyl ester (9CI) (CA INDEX NAME)



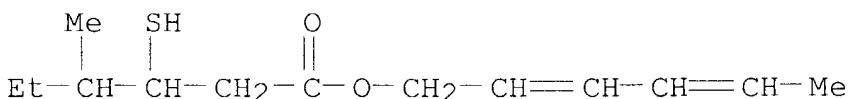
IC ICM A61K007-06
 ICS A61K007-09; A61K007-155; C14C001-06
 CC 62-3 (Essential Oils and Cosmetics)
 Section cross-reference(s): 45
 IT 26473-47-2 54051-19-3
 (cosmetic depilatories and waving prepns. and hide dehairing prepns. contg.)

L39 ANSWER 4 OF 5 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1975:427629 HCPLUS
 DOCUMENT NUMBER: 83:27629
 TITLE: β -Mercaptoalkanoates for perfumes and flavorants
 INVENTOR(S): Helmlinger, Daniel; Lamparsky, Dietmar; Schudel, Peter; Sigg-Gruetter, Trudi; Wild, Jost
 PATENT ASSIGNEE(S): Givaudan, L., et Cie. S. A.
 SOURCE: Patentschrift (Switz.), 4 pp. Division of Swiss 545,775 (See Ger. 2,155,672, CA 77: 100835j).
 CODEN: SWXXAS
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 557423	A	19741231	CH 1973-3097	19701211
PRIORITY APPLN. INFO.:			CH 1973-3097	19701211
AB HSCHRCH ₂ CO ₂ R ₁ (I; R = pentyl, hexyl, heptyl, 1-heptenyl, EtCHMe, or Et ₂ CH; R ₁ = Me, Et, cis-3-hexenyl, 2-hexenyl, or 2,4-hexadienyl), with fruity or flower-like odors were prepd. Thus, addn. of H ₂ S to 50 g EtCMe:CHCO ₂ Et gave, after purification, 47 g I (R = EtCHMe and R ₁ = Et), which had a light fruity aroma.				
IT	37486-70-7P 37549-67-0P 37549-82-9P 37549-84-1P (prepn. of)			
RN	37486-70-7 HCPLUS			
CN	Hexanoic acid, 3-mercaptop-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)			

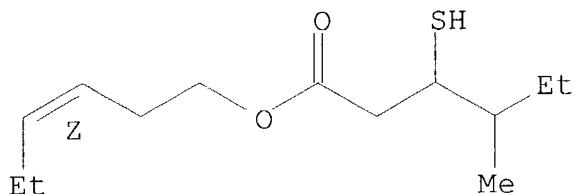


RN 37549-67-0 HCPLUS
 CN Hexanoic acid, 3-mercaptop-4-methyl-, 2,4-hexadienyl ester (9CI) (CA INDEX NAME)

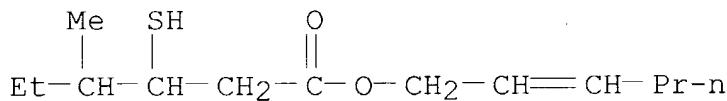


RN 37549-82-9 HCPLUS
 CN Hexanoic acid, 3-mercaptopro-4-methyl-, 3-hexenyl ester, (Z)- (9CI)
 (CA INDEX NAME)

Double bond geometry as shown.



RN 37549-84-1 HCPLUS
 CN Hexanoic acid, 3-mercaptopro-4-methyl-, 2-hexenyl ester (9CI) (CA INDEX NAME)



IC C11B; A23L
 CC 23-18 (Aliphatic Compounds)
 Section cross-reference(s): 62
 ST mercaptoalkanoate **perfume flavoring** agent;
 alkanoate mercapto **perfume flavorant**
 IT **Flavoring** materials
Perfumes
 (mercaptoalkanoates for)
 IT Esters, preparation
 (of β -mercaptoalkanoic acids, with fruity or flower-like
 aromas)
 IT 928-96-1P 37486-70-7P 37549-67-0P 37549-75-0P
 37549-76-1P 37549-77-2P 37549-78-3P 37549-79-4P 37549-81-8P
 37549-82-9P 37549-83-0P 37549-84-1P
 (prepn. of)

L39 ANSWER 5 OF 5 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1972:500835 HCPLUS
 DOCUMENT NUMBER: 77:100835
 TITLE: Alkyl-and alkenyl 3-mercaptopropionates
 INVENTOR(S): Helmlinger, Daniel; Lamparsky, Dietmar; Schudel,
 Peter; Sigg-Gruetter, Trudi; Wild, Jost
 PATENT ASSIGNEE(S): Givaudan, L., et Cie. S. A.

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2155672	A	19720629	DE 1971-2155672	19711109
DE 2155672	B2	19800508		
DE 2155672	C3	19810129		
CH 545775	A	19740215	CH 1970-18383	19701211
NL 7115451	A	19720613	NL 1971-15451	19711110
BE 776520	A1	19720612	BE 1971-111513	19711210
FR 2117625	A5	19720721	FR 1971-44385	19711210
GB 1336037	A	19731107	GB 1971-57456	19711210

PRIORITY APPLN. INFO.: CH 1970-18383 19701211

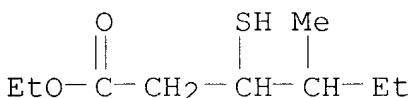
AB Nine R₁CH(SH)CH₂CO₂R [I, R = Et, Me, (CH₂)₂CH:CHEt, CH:CHBu, CH₂(CH:CH)2Me: R₁ = C₄₋₇ alkyl or CH:CH(CH₂)₄Me], used as **odorous substances in perfumes**, were prep'd. by autoclaving R₁CH:CHCO₂R with H₂S in alcs. in the presence of Na alkoxides or KOH or NaOH and hydroquinone or azobisisobutyronitrile. The compn. of a lavender-type **perfume** contg. I (R = Et, R₁ = CHMeEt) was reported.

IT 37486-70-7P 37549-67-0P 37549-82-9P
37549-84-1P

(prepn. of)

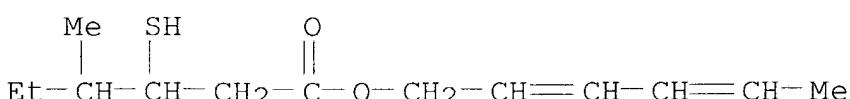
RN 37486-70-7 HCPLUS

CN Hexanoic acid, 3-mercaptop-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



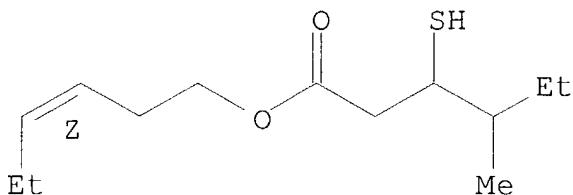
RN 37549-67-0 HCPLUS

CN Hexanoic acid, 3-mercaptop-4-methyl-, 2,4-hexadienyl ester (9CI) (CA INDEX NAME)

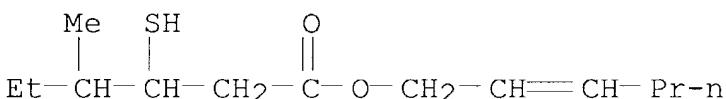


RN 37549-82-9 HCPLUS
 CN Hexanoic acid, 3-mercaptopro-4-methyl-, 3-hexenyl ester, (Z)- (9CI)
 (CA INDEX NAME)

Double bond geometry as shown.



RN 37549-84-1 HCPLUS
 CN Hexanoic acid, 3-mercaptopro-4-methyl-, 2-hexenyl ester (9CI) (CA INDEX NAME)



IC C07C; C11B; A23L
 CC 23-17 (Aliphatic Compounds)
 Section cross-reference(s): 62
 ST perfume mercapto ester aliph; hydrogen sulfide addn
 olefinic ester
 IT **Perfumes**
 (mercapto aliphatic esters for)
 IT 37486-70-7P 37549-66-9P 37549-67-0P
 37549-75-0P 37549-76-1P 37549-77-2P 37549-78-3P 37549-79-4P
 37549-80-7P 37549-81-8P 37549-82-9P 37549-83-0P
 37549-84-1P 37645-98-0P
 (prepn. of)

=> d 140 1-6 cbib abs hitstr hitind

L40 ANSWER 1 OF 6 HCPLUS COPYRIGHT 2004 ACS on STN
 2002:808766 Document No. 138:170279 Synthetic equivalents of
 benzenethiol and benzyl mercaptan having faint **smell**:
odor reducing effect of trialkylsilyl group. Nishide,
 Kiyoharu; Miyamoto, Tetsuo; Kumar, Kamal; Ohsugi, Shin-ichi; Node,
 Manabu (Kyoto Pharmaceutical University, Misasagi, Yamashina, Kyoto,
 607-8414, Japan). Tetrahedron Letters, 43(47), 8569-8573 (English)
 2002. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT

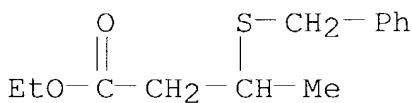
138:170279. Publisher: Elsevier Science Ltd..

AB Syntheses and **odor** tests of the 4-RC₆H₄X, 3-RC₆H₄X and 2-C₆H₄X (R = Me₃Si, Et₃Si, Pr₃Si; X = SH, CH₂SH) have revealed that the trimethylsilyl substituent on the benzene ring has a remarkable effect in reducing the foul **smell** of the parent benzyl mercaptan and benzenethiol. Protodesilylation allowed these silylated thiols to function as **odorless** synthetic equiv. of benzyl mercaptan and benzenethiol. The 4-Me₃Si-substituted benzenethiol and benzyl mercaptan were tested as nucleophiles in Michael addn. reactions with R₁HC:CR₃COR₄ (R₄ = OEt; R₁, R₃ = H or Me; R₄ = Et, R₁ = Me, R₃ = H) followed by protodesilylation to give corresponding phenylthio and phenylthiomethyl derivs. Radical addn. to PhC.tplbond.CCO₂Et and 2-nitropropionate redn. reactions were also tested. Nucleophilic substitution of Br in 1-bromo-3-phenylpropane by 4-Me₃SiC₆H₄SH was followed by halodesilylation, affording 4-iodo- and 4-bromo- derivs. This discovery will greatly improve the phys. environment of the researcher working with these malodorous compds.

IT 89529-96-4P 111731-00-1P
(Michael addn. product; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

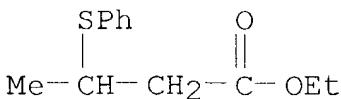
RN 89529-96-4 HCAPLUS

CN Butanoic acid, 3-[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



RN 111731-00-1 HCAPLUS

CN Butanoic acid, 3-(phenylthio)-, ethyl ester (9CI) (CA INDEX NAME)

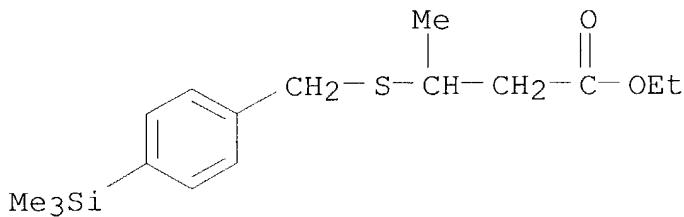


IT 497181-03-0P 497181-04-1P

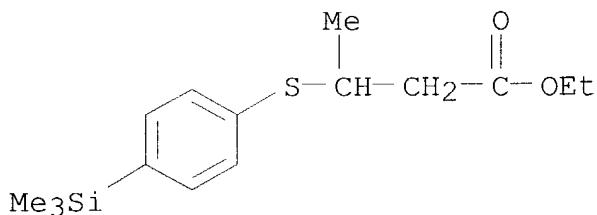
(protodesilylation; nucleophilic Michael addn. of silylated synthetic equiv. of benzyl mercaptans and thiophenols with subsequent protodesilylation)

RN 497181-03-0 HCAPLUS

CN Butanoic acid, 3-[[[4-(trimethylsilyl)phenyl]methyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)



RN 497181-04-1 HCAPLUS
 CN Butanoic acid, 3-[(4-(trimethylsilyl)phenyl)thio]-, ethyl ester
 (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 21
 ST benzenethiol benzylmercaptan synthetic equiv silyl deriv low
odor prep; silane deriv thiophenol benzenemethanethiol
 desilylation protonolysis bromination iodination; Michael
 condensation propiolate addn nucleophilic substitution silyl
 modified thiol; nucleophilic reaction silyl modified thiol low
odor desilylation; thiol synthetic equiv nucleophilic
 reaction low **odor** product deprotection; green chem thiol
 mercaptan synthetic equiv low **odor**
 IT Hydrolysis
 (acid, protodesilylation; prep. of low-**odor** silylated
 synthetic equiv. of benzyl mercaptans and thiophenols, their
 nucleophilic reactions and desilylation)
 IT Bromination
 (bromodesilylation; prep. of low-**odor** silylated
 synthetic equiv. of benzyl mercaptans and thiophenols, their
 nucleophilic reactions and desilylation)
 IT Substituent effects
 (effect of trialkylsilyl substituent on **odor** of
 benzenethiols and benzyl mercaptans)
 IT Iodination
 (iododesilylation; prep. of low-**odor** silylated

synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT Odor and Odorous substances
(nucleophilic Michael addn. of silylated synthetic equiv. of benzyl mercaptans and thiophenols with subsequent protodesilylation)

IT Thiols (organic), preparation
(odor scale, Michael addn., redn., nucleophilic substitution; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT Green chemistry
Michael reaction
Silylation
Substitution reaction, nucleophilic
(prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT Addition reaction
(radical; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT Silylation
(retro; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 60805-64-3P 89529-96-4P 111731-00-1P
241480-19-3P 377092-98-3P 497181-08-5P 497181-09-6P
497181-10-9P
(Michael addn. product; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 57337-85-6P
(Michael addn., odor scale; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 497180-93-5P 497180-94-6P 497180-95-7P
(Newman-Kwart rearrangement, thiolation; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 995-25-5
(arylation; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 13132-25-7 15288-53-6 17881-95-7
(carbamothioic acid esterification; prepn. of low-odor silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 30134-12-4P 497181-12-1P 497181-13-2P 497181-14-3P
 (desilylation; prepn. of low-**odor** silylated synthetic
 equiv. of benzyl mercaptans and thiophenols, their substitution
 reactions and desilylation)

IT 17882-12-1P
 (**odor** scale, Michael addn., radical addn., redn.,
 desilylation; prepn. of low-**odor** silylated synthetic
 equiv. of benzyl mercaptans and thiophenols, their nucleophilic
 reactions and desilylation)

IT 17881-83-3P 33356-45-5P 497180-78-6P 497180-79-7P
 497180-80-0P 497180-81-1P 497180-82-2P 497180-83-3P
 497180-84-4P 497180-85-5P
 (**odor** scale; prepn. of low-**odor** silylated
 synthetic equiv. of benzyl mercaptans and thiophenols, their
 nucleophilic reactions and desilylation)

IT 95-56-7, 2-Bromophenol 106-41-2, 4-Bromophenol 591-20-8,
 3-Bromophenol 994-30-9, Chlorotriethylsilane
 (prepn. of low-**odor** silylated synthetic equiv. of
 benzyl mercaptans and thiophenols, their nucleophilic reactions
 and desilylation)

IT 497180-99-1P 497181-00-7P 497181-01-8P 497181-02-9P
497181-03-0P 497181-04-1P 497181-05-2P
 497181-06-3P 497181-07-4P
 (protodesilylation; nucleophilic Michael addn. of silylated
 synthetic equiv. of benzyl mercaptans and thiophenols with
 subsequent protodesilylation)

IT 20591-87-1P
 (redn. product; prepn. of low-**odor** silylated synthetic
 equiv. of benzyl mercaptans and thiophenols, their addn. and
 redn. reactions and desilylation)

IT 2531-80-8
 (redn.; prepn. of low-**odor** silylated synthetic equiv.
 of benzyl mercaptans and thiophenols, their addn. and redn.
 reactions and desilylation)

IT 497180-96-8P 497180-97-9P 497180-98-0P
 (redn.; prepn. of low-**odor** silylated synthetic equiv.
 of benzyl mercaptans and thiophenols, their nucleophilic
 reactions and desilylation)

IT 95-46-5 106-38-7 591-17-3
 (silylation; prepn. of low-**odor** silylated synthetic
 equiv. of benzyl mercaptans and thiophenols, their nucleophilic
 reactions and desilylation)

IT 637-59-2
 (thioetherification; prepn. of low-**odor** silylated
 synthetic equiv. of benzyl mercaptans and thiophenols, their
 substitution reactions and desilylation)

IT 17903-42-3 17903-43-4 17903-44-5
 (thiolation; prepn. of low-**odor** silylated synthetic

equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 19061-64-4P 497180-86-6P 497180-87-7P 497180-88-8P
 497180-89-9P 497180-90-2P
 (thiolation; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

IT 497181-11-0P
 (thiophenol addn. product; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT 2216-94-6, Ethyl phenylpropiolate
 (thiophenol radical addn.; prepn. of low-**odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their addn. and redn. reactions and desilylation)

IT 3644-91-5 18412-77-6 18412-78-7
 (α -bromination; prepn. of low- **odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

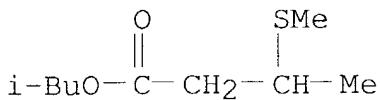
IT 3728-43-6P 3728-44-7P 7450-03-5P 17897-71-1P 497180-91-3P
 497180-92-4P
 (α -bromination; prepn. of low- **odor** silylated synthetic equiv. of benzyl mercaptans and thiophenols, their nucleophilic reactions and desilylation)

L40 ANSWER 2 OF 6 HCPLUS COPYRIGHT 2004 ACS on STN
 1990:439170 Document No. 113:39170 Alkyl (3-methylthio)-butyrates, their preparation and use as fruit **flavoring** agents.
 Bruijnje, Arnold; Heideman, Theo; Wille, Hans Julius (Naarden International N. V., Neth.). Eur. Pat. Appl. EP 330254 A1 19890830, 6 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1989-200313 19890210. PRIORITY: NL 1988-502 19880226.

AB $\text{CH}_3\text{CH}(\text{SH})\text{CH}_2\text{CO}_2\text{R}$ ($\text{R} = \text{C}_4\text{-5}$ optionally branched alkyl) is manufd. and used as a **flavoring** agent imparting fresh fruit **flavor**. Thus, iso-Bu (3-methylthio)-butyrate (I) was prep'd. from Na methoxide, isobutylcrotonate, and methylmercaptan with a yield of 88%. Prepn. of a strawberry **flavor** compn. contg. I and its use in manufg. strawberry jam were also disclosed.

IT 127931-21-9P
 (manuf. of, as fruit **flavoring** agent)

RN 127931-21-9 HCPLUS
 CN Butanoic acid, 3-(methylthio)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



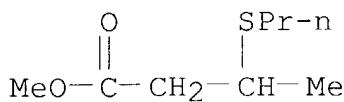
IC ICM C07C149-20
ICS A23L001-226
CC 17-6 (Food and Feed Chemistry)
ST butyrate fruit **flavor** agent manuf; strawberry
flavor butyrate
IT **Flavoring** materials
(fruit, alkylmethylthiobutyrates, prepn. and use of)
IT **Flavoring** materials
(strawberry, isobutylmethylthio butyrate, prepn. and use of)
IT Jams and Jellies
(strawberry, strawberry-**flavored**, manuf. of,
isobutylmethylthio butyrate prepn. in relation to)
IT Milk preparations
(yogurt, strawberry-**flavored**, manuf. of,
isobutylmethylthio butyrate prepn. in relation to)
IT 74-93-1, Methylmercaptan, biological studies 124-41-4 589-66-2,
Isobutylcrotonate
(in **flavoring** agent butyrate manuf.)
IT 127931-21-9P
(manuf. of, as fruit **flavoring** agent)

L40 ANSWER 3 OF 6 HCPLUS COPYRIGHT 2004 ACS on STN
1987:195056 Document No. 106:195056 Esters of alkylthioalkanoic acids
as **aromas** and **flavors** for foods. Courtney,
Thomas F., Jr.; Pittet, Alan O.; Muralidhara, Ranya; Vock, Manfred
H.; Wiener, Charles (International Flavors and Fragrances Inc.,
USA). U.S. US 4631194 A 19861223, 49 pp. (English). CODEN:
USXXAM. APPLICATION: US 1985-789162 19851206.

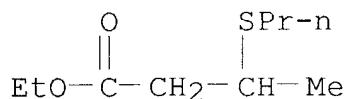
AB The **aroma** and **taste** of foods are enhanced by
addn. of 0.001-250 ppm (by wt. of the food) of an ester of an
alkylthioalkanoic acid. Thus, allyl-2(3-
hydroxypropylthio)propionate, having a roasted, sesame **aroma**
and **taste** profile at 2 ppm, was prepd. by reaction of
2-mercaptopropionic acid with allyl alc. in the presence of
p-toluenesulfonic acid.

IT 108073-21-8P 108073-22-9P 108073-24-1P
108073-27-4P
(prepn. of, as food **aroma** and **flavor**
enhancer)

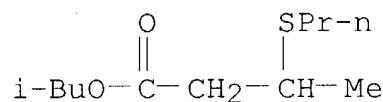
RN 108073-21-8 HCPLUS
CN Butanoic acid, 3-(propylthio)-, methyl ester (9CI) (CA INDEX NAME)



RN 108073-22-9 HCPLUS
CN Butanoic acid, 3-(propylthio)-, ethyl ester (9CI) (CA INDEX NAME)

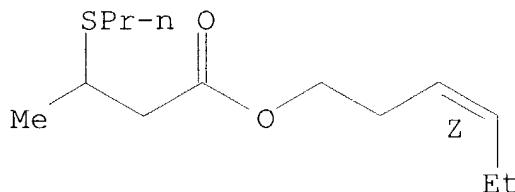


RN 108073-24-1 HCAPLUS
CN Butanoic acid, 3-(propylthio)-, 2-methylpropyl ester (9CI) (CA
INDEX NAME)



RN 108073-27-4 HCAPLUS
CN Butanoic acid, 3-(propylthio)-, 3-hexenyl ester, (Z)- (9CI) (CA
INDEX NAME)

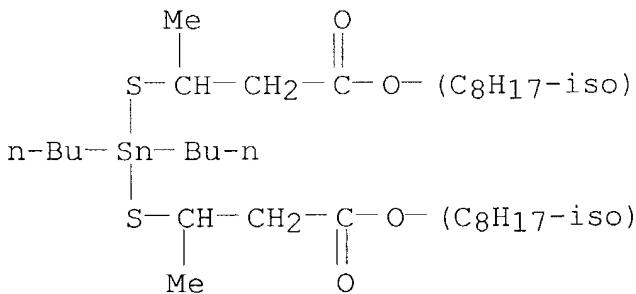
Double bond geometry as shown.



IC ICM A23L001-226
IC S ICS A23L001-231; A23L001-235
NCL 426535000
CC 17-6 (Food and Feed Chemistry)
ST alkylthioalkanoic acid ester food flavor aroma;
thioalkanoate alkyl ester food flavor aroma
IT **Flavoring** materials
 (alkylthioalkanoic acid esters)
IT **Odor** and **Odorous** substances

IT (alkylthioalkanoic acid esters, for food)
IT Carboxylic acids, esters
IT (alkylthio, esters, as **aroma** and **flavor**
IT substances for foods)
IT 90113-14-7P 108073-20-7P 108073-21-8P
IT 108073-22-9P 108073-23-0P 108073-24-1P
IT 108073-25-2P 108073-26-3P 108073-27-4P 1
IT 108073-29-6P
IT (prepn. of, as food **aroma** and **flavor**
IT enhancer)

L40 ANSWER 4 OF 6 HCPLUS COPYRIGHT 2004 ACS on STN
1970:112263 Document No. 72:112263 Organotin stabilizers. Stapfer,
Christian H. (Carlisle Chemical Works, Inc.). Fr. FR 1578260
19690814, 7 pp. (French). CODEN: FRXXAK. PRIORITY: US 19670719.
AB Dibutyltin azelate (I) or bis[(carbisoctoxymethylthio)dibutyltin]
azelate and dibutyltin bis(isooctyl mercaptoacetate) (II) or
dibutyltin bis(isooctyl 3-mercaptopropionate) are used as efficient
internal lubricants having no undesirable **odor** during
extrusion of poly(vinyl chloride) (III). Thus, III contg. 0.5% I
and 1.5% II had an extrusion index of 42 kg/hr as compared with 36.6
kg/hr for III contg. 2.5% II.
IT 26898-05-5
(stabilizers, for vinyl chloride polymers, internal lubrication
in relation to)
RN 26898-05-5 HCPLUS
CN Butyric acid, 3,3'-(dibutylstannylene)dithio]di-, diisooctyl ester
(8CI) (CA INDEX NAME)



IC C07F; C08F
CC 36 (Plastics Manufacture and Processing)
IT 25168-24-5 **26898-05-5** 26898-06-6 27468-47-9
 (stabilizers, for vinyl chloride polymers, internal lubrication
 in relation to)

L40 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

1957:40568 Document No. 51:40568 Original Reference No. 51:7607f-i

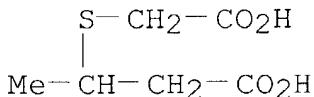
The **flavor** problem of soybean oil. XIII. Sulfur coordination compounds effective in edible-oil stabilization. Schwab, A. W.; Moser, Helen A.; Gurley, Rosemary S.; Evans, C. D. (Northern Regional Research Lab., Peoria, IL). J. Am. Oil Chemists' Soc., 30, 413-17 (Unavailable) 1953.

AB cf. C.A. 47, 6569f. S compds. of the tridentate class having at least 2 COOH groups in α - or β -position to the coordinate atom are effective in stabilization of soybean oil. Among comparative model compds. with different coordinating atoms, the order of effectiveness appears to be S > N > O. (Carboxymethylthio)butyric acid, (carboxymethylthio)phenylpropionic acid, the monoethyl ester of (carboxymethylthio)succinic acid, p-toluenesulfonic acid, α, α' -thiodicaproic acid, and SO₂ all improve the oxidative stability but gave undesirable **flavors**. Thiodiacetic acid, β, β' -thiodipropionic acid, (carboxymethylthio)succinic acid (I), and monooctadecyl ester of I were excellent stabilizers. The first 2 can be added either on the upgrade or the downgrade of deodorization, but the heat stability of the latter 2 limits their addn. to the downgrade. All these compds. improved the **flavor** stability as well as the oxidative stability. The monooctadecyl ester has the added advantage in that it is oil-sol.

IT 4386-05-4, Butyric acid, 3-(carboxymethylthio)- (soybean oil **flavor** and oxidative stabilization by)

RN 4386-05-4 HCPLUS

CN Butanoic acid, 3-[(carboxymethyl)thio]- (9CI) (CA INDEX NAME)



CC 12 (Foods)

IT Soybean oil

(**flavor** and oxidative stabilization of, S coordination compds. in)

IT 99-68-3, Succinic acid, (carboxymethylthio)- (and esters, soybean oil **flavor** and oxidative stabilization by)

IT 7704-34-9, Sulfur (compds., soybean oil **flavor** and oxidative stabilization by)

IT 104-15-4, p-Toluenesulfonic acid 111-17-1, Propionic acid, 3,3'-thiodi- 123-93-3, Acetic acid, thiodi- 505-47-5, Propionic acid, 3,3'-iminodi- 4386-05-4, Butyric acid, 3-(carboxymethylthio)- 5961-83-1, Propionic acid, 3,3'-oxydi-

67242-91-5, Hydrocinnamic acid, β -(carboxymethylthio)-
105910-65-4, Hexanoic acid, 2,2'-thiodi-
(soybean oil flavor and oxidative stabilization by)

L40 ANSWER 6 OF 6 HCPLUS COPYRIGHT 2004 ACS on STN
1957:1799 Document No. 51:1799 Original Reference No. 51:395b-i, 396a-d
The thiazole series. III. Sulfur-heterocyclic derivatives of
2-aminothiazole. Cagnoli, Nerina; Ricci, Adolfo (Univ. Perugia,
Italy). Annali di Chimica (Rome, Italy), 46, 275-82 (Unavailable)
1956. CODEN: ANCRAI. ISSN: 0003-4592.

GI For diagram(s), see printed CA Issue.

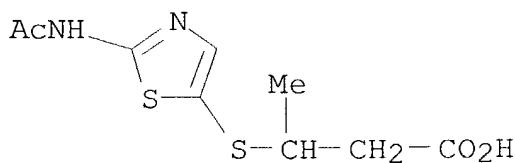
AB cf. C.A. 46, 496i; 50, 5564c. A number of derivs. have been prepd. from 2-amino-5-thiocyanothiazole, which has been prepd. from 2-aminothiazole and HSCN (C.A. 46, 496i). Thus, (2-acetamidothiazole-5-thio)propionic acid (I), white crystals, m. 185° (from alc.), was prepd. by adding 10 g. of (2-acetamido-5-thio)cyanothiazole (II) slowly to a freshly prepd. aq. soln. of 12 g. Na₂S, heating to complete soln., cooling, decolorizing, and filtering off 2-acetamido-5-mercaptopthiazole (III), which pptd. upon acidifying, redissolving 10 g. III in 2.3 g. NaOH in water, adding 9 g. BrCH₂CH₂CO₂H, heating briefly until the color was light yellow, cooling, and pptg. by adding acid. I was also prepd. by adding 10 g. II to an aq. alc. soln. of 4 g. NaOH, heating to dissolve, adding an alk. soln. of 7.7 g. BrCH₂CH₂CO₂H, heating until the reddish color lightened, cooling, and acidifying. Hydrolysis of I yielded (2-aminothiazole-5-thio)propionic acid, needles, m. 200-201° (from H₂O). S.CHR.CH₂.CO.C:C.S.C(NH₂):N (IV) (R = H), straw-colored needles, m. 240-1°, formed when 2 g. of I was dissolved in 10 ml. concd. H₂SO₄, heated to 60-70° for 1 hr., poured into H₂O pptg. the product, which was filtered off, and washed with H₂O and Na₂CO₃ soln. The diazo deriv. of IV coupled with PhNMe₂ yielded a dark red dye, m. 228-9° (from MeOH). Other derivs. were 2-acetyl-IV (R = H), white silky needles, m. 255-6° (from alc.), and IV-thiosemicarbazone (R = H), shiny whitish needles, m. 230-1° (from alc.), prepd. by dissolving 1 g. IV in a little alc., adding a few drops of 30% alc. HCl, heating, adding 0.5 g. thiosemicarbazide, heating, and collecting the ppt. for purification. β -Methyl(2-acetamidothiazole-5-thio)propionic acid (V), C₉H₁₂O₃N₂S₂, white silky needles, m. 188-9° (from H₂O), was made from II and β -bromobutyric acid as described above. IV (R = Me) (VI), yellow needles, m. 269-70° (decompn.) (from alc.) was likewise prepd. from V. 2-Acetyl-VI, needles, m. 288-9°, sol. in NaOH. VI thiosemicarbazone, m. 252-3° (from alc.). (2-Acetamidothiazole-5-thio)propanediol, white crystals, m. 165-6°, was prepd. by dissolving 10 g. III and 2.3 g. NaOH in hot alc. and adding 6.5 g. glycerol α -monochlorohydrin and heating 2 hrs., cooling, filtering off

the product and crystg. it from alc. The product was hydrolyzed to (2-aminothiazole-5-thio)propanediol, white needles, m. 115-16° (from H₂O). S.C(NHAc):N.CH:CSC₆H₃(CO₂H)NO₂-2,4 (VII), obtained as its Na salt, golden-yellow scales, m. 322-3°, was prep'd. from 10 g. III, and 2.3 g. NaOH in alc., 5 g. NaHCO₃, and 11.6 g. 2-chloro-5-nitrobenzoic acid in alc. by refluxing 2 hrs., cooling, collecting the ppt'd. Na salt, and crystg. from hot H₂O. The 2-H₂N analog, yellow crystals, m. 257-8° (from alc., decompn.), was prep'd. by acid hydrolysis of VII. VIIa, orange-yellow needles, m. 340°, was prep'd. by treating VII with 10 ml. concd. H₂SO₄ and 2 g. P₂O₅ for 1 hr. at 70-80°, leaving overnight, pouring into ice, collecting the ppt., washing with Na₂CO₃, drying at 80°, and crystg. from PhNO₂. 4-Oxo-2-acetamido-4,5-dihydrothieno[2,3-b]thiazole, white crystals, m. above 320°, was prep'd. (1 g. yield) by suspending 10 g. S-(2-acetamido-5-thiazolyl)thioglycolic acid in 50 ml. POC₁₃ and refluxing 2-3 hrs., distilling off the excess POC₁₃, pouring into ice water, neutralizing with Na₂CO₃, and collecting the brick-red ppt. from AcOH. 2-Acetamido-5-thiazolyl 2-nitrophenyl sulfide (VIII), white needles, m. 225-6° (from alc.), was prep'd. by adding 10 g. III to an alc. soln. of 2.3 g. NaOH, taking to a boil, adding 7.2 g. 2-ClC₆H₄NO₂ in alc., refluxing 4 hrs., cooling, distg. off most of the alc., collecting the ppt., and crystg. from alc. 2-Acetamido-5-thiazolyl 2-aminophenyl sulfide, bunches of white needles, m. 217-18° (from alc.), was prep'd. by suspending 10 g. VIII in a little alc., adding 50 ml. NH₄OH and 20 ml. H₂O, heating to 60-70°, adding a soln. of 66 g. FeSO₄ in water, agitating 1 hr., filtering the cooled soln., extg. the ppt. with hot alc., and purifying by extg. with dil. HCl and repptg. Diazotized and decompd., this yielded a product, m. 120-4°, with an odor resembling that of PhNO₂ (cf. Cullinane, et al., C.A. 31, 3987). 2-Acetamido-5-thiazolyl 2,4-dinitrophenyl sulfide, yellow needles, m. 294-5° (from alc.), was prep'd. from 10 g. III, 2.3 g. NaOH, and 11.6 g. 2,4-(O₂N)C₆H₃Cl in the described manner. VIIa, small shiny crystals, m. 247-8°, was prep'd. by dissolving 5 g. 3-methyl-5-aminothianaphthene in a little AcOH, cooling to 0°, and adding slowly 1.75 ml. Br₂ in AcOH. Thiocyanation yielded a white cryst. material which is poured into H₂O, neutralized with Na₂CO₃, and crystd. from alc.

IT 99362-84-2, Butyric acid, 3-(2-acetamido-5-thiazolylthio)-
(prepn. of)

RN 99362-84-2 HCPLUS

CN Butyric acid, 3-(2-acetamido-5-thiazolylthio)- (6CI) (CA INDEX
NAME)



CC 10 (Organic Chemistry)
 IT 98134-99-7, Propionic acid, 3-(2-amino-5-thiazolylthio)-
 98489-98-6, 1,2-Propanediol, 3-(2-acetamido-5-thiazolylthio)-
 99073-61-7, Benzoic acid, 2-(2-amino-5-thiazolylthio)-5-nitro-
99362-84-2, Butyric acid, 3-(2-acetamido-5-thiazolylthio)-
 99848-24-5, 1,2-Propanediol, 3-(2-amino-5-thiazolylthio)-
 99973-26-9, Thiazole, 2-acetamido-5-(o-nitrophenylthio)-
 99974-43-3, Thiazole, 2-acetamido-5-(2,4-dinitrophenylthio)-
 100377-69-3, Propionic acid, 3-(2-acetamido-5-thiazolylthio)-
 108249-46-3, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro-
 6-methyl-, thiosemicarbazone 108480-68-8, 7H-Thiopyrano[3,2-
 d]thiazol-7-one, 2-acetamido-5,6-dihydro- 108845-52-9,
 9H-[1]Benzothiopyrano[3,2-d]thiazol-9-one, 2-acetamido-7-nitro-
 110937-01-4, Thiazole, 2-acetamido-5-(o-aminophenylthio)-
 114794-02-4, 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro-
 6-methyl- 115247-56-8, Thieno[3,2-f]benzothiazole,
 2-amino-7-methyl- 117883-91-7, Benzoic acid, 2-(2-acetamido-5-
 thiazolylthio)-5-nitro-, sodium salt 119248-31-6,
 7H-Thiopyrano[3,2-d]thiazol-7-one, 2-amino-5,6-dihydro-,
 thiosemicarbazone 120208-30-2, Thieno[3,2-d]thiazol-6(5H)-one,
 2-acetamido- 120267-20-1, 7H-Thiopyrano[3,2-d]thiazol-7-one,
 2-amino-5,6-dihydro- 120944-93-6, 7H-Thiopyrano[3,2-d]thiazol-7-
 one, 2-acetamido-5,6-dihydro-5-methyl-
 (prep. of)